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EG&G ROCKY FLATS

INTEROFFICE CORRESPONDENCE

DATE: December 7, 1994

TO: S. G. Stiger, Environmental Restoration Program Division, Bldg. 080, X8540

FROM: F. W. Chromec, ERPD - Risk Assessment, Building 080, X8641, DP 5144 FWC

SUBJECT: REVIEW OF GROUNDWATER MODELING - FWC-004-94

DOE Order: 4700.1

Action: None required at this time

At staff Monday, November 7, I was tasked to deliver information on ground water modeling efforts at the Rocky Flats Environmental Technology Site. In response, three reports have been prepared concerning: OU– specific groundwater modeling; the site–wide groundwater model; and geochemical modeling.

The OU–specific report summarizes model codes used at the Rocky Flats Environmental Technology Site, hydrologic conditions and models chosen for several OUs. These models can not be directly linked for application to larger areas due to different grid sizes, large areas between simulations that have not been modeled, and different calibration sets. It may not be possible to combine individual OU modeling efforts to meet the requirements of DOE Order 5400.1 that an integrated overview of the Rocky Flats Environmental Technology Site be completed. A site–wide model would be more appropriate for both the Comprehensive Risk Assessment (CRA) and the Environmental Risk Assessment (ERA). However, due to schedule constraints it may be necessary to attempt to integrate individual OU models.

A site–wide model for the Rocky Flats Environmental Technology Site was developed in–house during fiscal year 1993 (FY93). The results of the modeling effort was presented in the 1993 Site–wide Groundwater Modeling Status Report. Products included site–wide bedrock and groundwater elevation maps and the first calibrated site–wide flow model. The model used a 200 foot grid spacing and did not include contaminant transport.

Work was planned for FY94 to expand and enhance the FY94 model. The work was in progress when direction came from the Department to Energy (DOE) to change the focus. In response, the area was reduced to include most of the industrial area and the Walnut and Women Creek drainages. A refined model was developed for this region that included a smaller, variable grid spacing and improved model calibration. The model was then used to perform particle tracking for the major groundwater flow paths. The results of this effort led to suggestions for thirteen additional monitoring locations.

ADMIN RECORD

The site-wide modeling efforts may be very useful for the ERA for OUs 5 and 6 and the Rocky Flats Environmental Technology Site CRA. Funding and personnel questions will need to be resolved for this to occur.

A summary of geochemical modeling efforts and a discussion of their potential uses is also included. These models will help to explain concentrations of inorganics in groundwater and predict their transport and behavior.

If you have any questions or comments on this report please do not hesitate to call me on extension 8641.

kld

Attachment
As Stated:

cc:
G. A. Anderson, w/o attachment
C. A. Bicher, w/o attachment
M. C. Broussard
M. S. Buddy, w/o attachment
W. S. Busby
M. C. Burmeister, w/o attachment
C. D. Cowdery, w/o attachment
T. R. DeMass, w/o attachment
D. R. Ferrier, w/o attachment
W. A. Fuller, w/o attachment
L. A. Gregory-Frost, w/o attachment
N. A. Holsteen, w/o attachment
J. K. Hopkins
R. Z. Houk, w/o attachment
W. M. Katz, w/o attachment
S. R. Keith
P. J. Laurin, w/o attachment
J. A. Ledford, w/o attachment
M. Z. Litaor, w/o attachment
E. C. Mast
M. F. McHugh, w/o attachment
J. B. Mellen, w/o attachment
K. K. O'Neill, w/o attachment
B. D. Peterman
L. J. Peterson-Wright, w/o attachment
A. L. Primrose
R. J. Ray, w/o attachment
D. A. Ringle, w/o attachment
D. L. Schubbe, w/o attachment
S. B. Smith, w/o attachment
ERPD Project File (2)

50016

Comparison of Operable Unit Groundwater Flow and Transport Modeling at the Rocky Flats Environmental Technology Site and Evaluation of Current Models for Use in Environmental Risk Assessment and Comprehensive Risk Assessment Studies

prepared for W. Chromec
Environmental Restoration Management
EG&G Rocky Flats, Inc.
Rocky Flats Environmental Technology Site
Golden, CO

Attachment 1
FWC-004-94

1.0 INTRODUCTION

Groundwater flow and transport modeling has a variety of uses at the Rocky Flats Environmental Technology Site (RFETS). Among these are the provision of concentration data for the Human Health Risk Assessment (HHRA), evaluation of various remediation/closure scenarios, and site characterization. A majority of the modeling completed thus far has been for the HHRA, but some modeling has been or is being completed for feasibility studies or closure stage.

2.0 OBJECTIVES

This document will describe the hydrogeologic conditions present at each OU, the types of modeling computer programs used, and the model construction parameters used. This document will also present an evaluation of the current modeling efforts to meet the needs of the Environmental Risk Assessment (ERA) and the Comprehensive Risk Assessment (CRA). Recommendations to meet the needs of the ERA and CRA are also presented.

3.0 MODELING

Modeling, in this document, is used to describe the set of activities involved with the simulation of the groundwater flow and contaminant transport using various mathematical equations and/or computer programs. The term 'model' is used to describe a picture of the site-specific hydrogeology formed by the hydrogeologist, computer programs used to perform the simulations, and the application of a computer program to a specific site.

A model has been described as a 'cartoon of reality'. It is important to remember when evaluating modeling that it is not reality. It is a simplification of our understanding of particular hydrogeologic systems (which is incomplete and based on a set of assumptions). Models are used to simulate the flow of groundwater and migration of contaminants in the subsurface. There are three types of models: conceptual, analytical, and numerical.

A conceptual model is a description of the primary processes that control the movement of groundwater and dissolved contaminants in the subsurface. This model is constructed by using diverse data sources collected in the field. These sources of data can include boring logs, water levels, pumping tests, groundwater flow rates and directions, solute release rates and timing, recharge and discharge rates, dispersion, chemical degradation rates, and adsorption.

The other types of models (analytical and numerical) involve the use of mathematical equations to simulate the flow and transport in a particular hydrogeologic conceptual model. Analytical solutions are exact solutions of the partial differential equations describing flow and transport for particular boundary conditions and assumptions. These boundary conditions should meet the description of the hydrogeology contained in the conceptual model. The most common assumptions used in analytical solutions include that the hydrogeologic system is homogeneous and isotropic. Where the hydrogeologic conditions are anisotropic and heterogeneous, a numerical model would be appropriate.

A numerical model is a computer program that will solve the descriptive partial differential equations for flow and transport. Using numerical techniques (most commonly finite difference and finite element), these equations can be solved for heterogeneous, anisotropic, and multi-layered hydrogeologic systems.

4.0 MODELING CODES USED AT RFETS

Several modeling codes at RFETS are used to simulate the hydrogeologic conditions at each OU. Modeling codes are selected to meet site conditions and project objectives. Modeling codes are selected using the following criteria:

1. The selected models should be able to incorporate key processes and accurately represent conditions known to occur at the site.

2. The selected models should be able to satisfy the objectives of the study.

3. The selected models should be verified using published equations and solutions.

4. The selected models should be complete and well documented and preferably available in the public domain.

5. The selected models should be practical and cost-effective in terms of actual application as well as resolution of uncertainty.

A variety of modeling codes are used at RFETS to meet the needs of the specific OU conditions and the needs of the particular project (HHRA, FS, etc.). Most of the site OUs have been or are being simulated using numerical modeling. There does appear to be a lack of groundwater and transport modeling in the Industrial Areas (with the exception of some analytical modeling in the Solar Ponds area). Descriptions of each of the modeling codes used at RFETS are presented below.

4.1. MODFLOW

MODFLOW is the U.S. Geological Survey's finite difference saturated flow model. This model is extensively used and well accepted by most regulatory agencies. It can simulate heterogeneous, multi-layered hydrogeologic systems. It can perform equilibrium and transient simulations. It is well documented (McDonald and Harbaugh, 1988) and has been verified and has produced numerically stable solutions (Anderson and Woessner, 1992). A series of 20 documented problems, four involving the use of analytical solutions, and their comparison to MODFLOW results has been published by the EPA (Anderson, 1993).

4.2. MT3D

MT3D is a proprietary numerical model released through S.S. Papadopolus and Associates. The source code of the model is provided with the documentation (Zheng, 1992). MT3D is a solute transport code that can integrate with the output from MODFLOW. It can, therefore, simulate heterogeneous, multi-layered contaminant transport systems under equilibrium and transient conditions. It can simulate a variety of transport processes such as sorption, radioactive decay, and biodegradation. Model verification is contained in chapter 7 of the model documentation.

4.3. PATH3D

PATH3D is a proprietary numerical model released through S.S. Papadopolus and Associates. PATH3D is a particle tracking code that can integrate with the output from MODFLOW. The model is capable of performing particle tracking in heterogeneous, multi-layered hydrogeologic systems under equilibrium and transient conditions. Particle tracking can be used to simulate the groundwater paths and travel times. Model verification is contained in the documentation (Zheng, 1989) and consists of the application of the model to example problems of varying complexity.

4.4. TARGET

TARGET is a proprietary numerical model released by Dames and Moore. Dames and Moore is in the process of releasing TARGET to the public through the International Ground Water Modeling Center in Golden, CO. TARGET can simulate both groundwater flow and contaminant transport in variably saturated conditions. Two- and three-dimensional, heterogeneous simulations can be performed under equilibrium and transient conditions.

4.5. Analytical Solutions

An analytical solution, as mentioned previously, is an exact solution of the partial differential equations describing groundwater flow and contaminant transport for a given set of boundary conditions. A variety of analytical solutions are used for work at RFETS. The analytical solutions are useful for relatively simple hydrogeologic systems or hydrogeologic systems that can be simplified. For an example of a published set of a variety of analytical solutions, the reader may consult Walton (1984).

5.0 HYDROGEOLOGIC DESCRIPTIONS OF RFETS OPERABLE UNITS

Modeling at RFETS has proceeded on an OU-by-OU basis and has depended on OU specific RI schedules. When modeling, no upgradient or adjacent contaminant sources are considered; only known sources within the OU are simulated. While this is not realistic, it does seek to meet the goals of the HHRA. There is an obvious need for a site-wide approach to evaluate the fate and transport of contaminants and their interactions, regardless of the OU in which they reside in. Sitewide modeling is the most applicable and appropriate for the ERA and CRA to be performed at RFETS.

The hydrogeologic layers at RFETS can be divided into an upper hydrostratigraphic unit (UHSU) and a lower hydrostratigraphic unit (LHSU). The UHSU is composed of the unconsolidated surficial deposits (Rocky Flats Alluvium, hillslope colluvium, and the valley fill alluvium) and the weathered bedrock (claystone and the Arapahoe Formation sandstones that outcrop or subcrop beneath the unconsolidated surficial deposits). The LHSU is composed of the unweathered bedrock (Laramie Formation claystone).

In order to examine the modeling approaches used at the various OUs at RFETS, it is necessary to briefly examine the hydrogeologic conditions at each OU. For a complete description of the hydrogeologic conditions present at each OU, the reader may consult the RCRA Facility Investigation/Remedial Investigation (RFI/RI) report for the particular OU.

5.1. OU1 Hydrogeologic Conditions

Groundwater flows beneath the 881 Hillside (the area of modeling concern) occurs in shallow colluvial, alluvial, and bedrock units. Most of the groundwater appears to be concentrated in the colluvium and valley-fill alluvium and is focused in areas where the colluvium is thickest. These areas generally correspond to surface-water drainages and are probably due to greater erosion and weathering of the bedrock beneath surface channels. The hydrogeologic system is variably saturated.

5.2. OU2 Hydrogeologic Conditions

The hydrogeologic conditions at OU2 are extremely complex. The complex subsurface geologic conditions dominate the hydrogeology, contaminant distribution, and transport within OU2. Due to the complex top-of-bedrock surface topography, and the influence of local precipitation as the dominant groundwater recharge mechanism, groundwater elevations and the areal extent of the saturated zone are highly variable during the year. This variability influences both the groundwater flow and contaminant distribution. Additionally, groundwater flow and transport are greatly influenced by the interaction between the saturated alluvium, the underlying bedrock, and the bedrock sandstone channel subcropping in OU2.

5.3. OU4 Hydrogeologic Conditions

The Solar Ponds are located on an alluvial terrace bench of alluvium, separating north and south Walnut Creek. The geology in OU4 is composed of the saturated alluvium, weathered bedrock (claystone), and the subcropping bedrock sandstones. Most of the groundwater in OU4 flows toward the northeast and southeast in the alluvial material. Groundwater seeps in the hillside above north Walnut Creek occurs where the bedrock contact subcrops. An extensive french drain system constructed in the unconsolidated materials modifies the groundwater flow system.

5.4. OU5 Hydrogeologic Conditions

OU5 consists of the Woman Creek drainage and groundwater occurs under unconfined conditions in the alluvium, weathered bedrock, colluvium, and valley fill alluvium. Several contaminant sources are present in several separate sources contained in the unsaturated zone. Most of these contaminant sources are within the old landfill and the ash pits.

5.5. OU6 Hydrogeologic Conditions

OU6 covers part of the Walnut Creek drainage and groundwater is likely to occur under unconfined conditions in the alluvium, colluvium, valley fill alluvium, and weathered bedrock claystones and sandstones subcropping against the alluvium. Limited areas of the subcropping claystone may be saturated, particularly where the claystones are fractured and weathered. Flow directions are generally from west to east, with local variations. Recharge to the unconfined water bearing zones is primarily due to precipitation, snowmelt, and water loss from ditches, streams, and ponds. Discharge appears to be from seeps and springs at the contact between the alluvium and the claystone bedrock. Contaminant sources appear to be mainly from other OUs and/or adjacent point sources. There does not appear to be a major groundwater contamination problem in OU6.

5.6. OU7 Hydrogeologic Conditions

The saturated groundwater system at OU7 (the present landfill) consists of the unconsolidated deposits overlaying the weathered bedrock (claystone). While both of these units make up the UHSU, most of the flow appears to be restricted to alluvial deposits. Fractures appear to be the dominant factor in the degree of saturation in the weathered bedrock unit. There are subsurface drain and slurry wall structures that affect subsurface groundwater flow. Recharge appears to be predominantly from precipitation and discharge is to the ponds, seeps, and streams in the area.

6.0 MODELING CONSISTENCY AT RFETS

Table 1 presents the hydrogeologic conditions present at each OU and the modeling code used for simulations of these hydrogeologic conditions. Examination of this table will reveal that modeling work at RFETS is consistent, where possible. Modeling codes are selected to simulate the particular conditions present at the individual OUs. Where conditions are roughly similar across OUs, the numerical modeling codes used are the same. It can be seen that most OUs are simulated using MODFLOW for groundwater flow and MT3D for contaminant transport. For the most part, the top surface of the bedrock is considered to be the base of the models (except where subcropping bedrock sandstones are present). Due to the impact of site activities in the UHSU and the low hydraulic conductivity of the bedrock claystones, there appears to be a very low level of hydraulic connection between the UHSU and the LHSU. Limited simulation of the bedrock claystones seems to agree with this conclusion. For this reason, the base of the UHSU is usually simulated as a no-flow boundary.

7.0 OPERABLE UNIT MODEL SUMMARIES

Table 2 presents the various parameters such as grid size, cell size and modeling codes used in the modeling activities for RFETS OUs. The most common use of HHRA modeling output is to provide the mass loading of contaminants to surface water modeling. FS modeling output is used to evaluate the 'best' scenario or scenarios for remedial alternatives or facility closures.

8.0 POTENTIAL USE OF MODELS FOR ERA AND CRA

Because of the OU-by-OU approach used in the HHRA and FS modeling, contaminant sources outside the OU are not considered, even when these contaminants are present in the OU being simulated. The OU models cannot be directly linked to form a sitewide model. Factors that preclude this include the use of different models at some OUs, differing grid sizes, large areas between the simulations that were not modeled, and different calibration sets.

The OU-by-OU approach is necessary in that the use of a sitewide scale model would tend to under-model (or average) the site-specific hydrogeology. In other words, the grid cell sizes for a sitewide model would probably be much larger and not provide the level of detail necessary to design OU-specific remediation approaches. To simulate the entire site, a level of detail is unnecessary that would be required for simulating an individual OU.

DOE Order 5400.1 requires that a comprehensive, integrated overview of RFETS be completed. It is obvious that the current modeling approach (OU-by-OU) does not meet this requirement. The ERA[1] and CRA are sitewide activities and a sitewide model would be the most useful and appropriate for this work. A sitewide model would also meet the requirements of DOE Order 5400.1. Due to schedule restraints, it is necessary that the results of the individual OU modeling be integrated to meet the requirements of the ERA. The CRA has not been initiated, and it would be appropriate to revive the existing sitewide model.

[1]The ERA will actually be implemented using a drainage basin approach.

The sitewide model could be used to integrate and evaluate contaminant transport across the entire site, considering all contaminant contributions from each OU to meet the requirements of DOE Order 5400.1 and the CRA (and the ERA, if possible). A sitewide model would also provide simulation of the groundwater and transport processes in the Industrial Area (which has not been done).

9.0 RECOMMENDATIONS

The results of the OU models may not be adequate to construct a sitewide model for the ERA and CRA because they will be difficult to integrate. Therefore, the following recommendations are presented:

1. Continue the sitewide modeling task. The current sitewide model should be further calibrated and expanded to include contaminant transport and fate. The model could then be used to support the CRA. If possible, the results from this model could then be used for the ERA, depending on schedule requirements.

2. Integration the results of the individual OU modeling (both groundwater and surface water, as well as air modeling), into a product that will be useful for the ERA. However, it may be necessary to hire a subcontractor to perform this task.

10.0 REFERENCES

Anderson, M.P. and W.W. Woessner. 1992. Applied Groundwater modeling. Academic Press, Inc., San Diego, CA.

Anderson, P.F. 1993. A manual of instructional problems for the U.S.G.S. MODFLOW model. U.S. Environmental Protection Agency, Robert S. Kerr Environmental Research Laboratory, Ada, OK.

EG&G Rocky Flats, 1993, Status Report: Site-wide groundwater flow modeling at the Rocky Flats Plant, Golden, Colorado.

McDonald, M.G. and A.W. Harbaugh. 1988. Techniques of water resources investigation of the United States Geological Survey, Book 6, Chapter A1, A modular three-dimensional finite-difference groundwater flow model.

Walton, W.C.. 1984. Handbook of analytical ground water models. International Ground Water Modeling Center, Indianapolis, IN[2].

Zheng, C. 1989. PATH3D. S.S. Papadopulos and Associates, Inc. Bethesda, Maryland.

Zheng, C. 1992. MT3D. S.S. Papadopolus and Associates, Inc. Bethesda, Maryland.

[2]The IGWMC is now located at the Colorado School of Mines in Golden. CO.

Table 1
RFETS Operable Unit Modeling
Operable Unit Modeling Consistency

NEED	OU1	OU2	OU5	OU6	OU7	Sitewide
Complex, Saturated Flow		MODFLOW	MODFLOW		MODFLOW	MODFLOW
Complex, 3D Saturated Transport		MT3D	MT3D			MT3D
Simple Flow and Transport		ONED3	Analytical Solution	ONED3 other Analytical Solutions		
Particle Tracking					PATH3D	PATH3D
Unsaturated Flow and Transport	TARGET					

Table 2
RFETS Operable Unit Modeling
Operable Unit Numerical Flow and Transport Model Descriptions

Parameters	OU1	OU2	OU2[1]	OU4	OU5	OU6	OU7	Sitewide Flow (1993)	Sitewide Flow and Particle Tracking (1994)
Model(s)	TARGET	MODFLOW MT3D	MODFLOW MT3D	Analytical	MODFLOW MT3D	Analytical[2]	MODFLOW PATH3D	MODFLOW	MODFLOW PATH3D
No. of Layers	3	1	2	1	1	?	2	1	1
Temporal Domain[3] (flow/transport)	Steady State /Transient	Steady State /Transient	Transient /Transient	Steady State /Transient	Steady State /Transient	Steady State /Transient	Steady State /Transient	Steady State	Steady State /Transient
Type of Model	2D Profile	2D Areal	3D	3D	2D Areal	?	3D	2D Areal	2D Areal
Grid Size (rows x cols)	296 x 170	16 x 46	?	n/a	155 x 24	n/a	100 x 30	74 x 92	94 x 122
Grid Cell Size (ft)	1 - 20	50 - 100	?	n/a	50 - 100	n/a	50	200	75 - 200
Model Size (ft)	880 x 230	4600 x 800	?	n/a	15000 x 1450	n/a	5000 x 1500	18400 x 14800	12150 x 10800
Purpose	HHRA	HHRA	FS	?	HHRA	HHRA	Landfill closure	General	1994 Well Evaluation Report
Completed?	Yes	Yes	No	Yes	No	No	No	Yes	Yes

Notes:
Completed modeling activities are documented in the RFI/RI reports for the appropriate OU.

[1]This model is currently being developed and the simulation parameters are subject to change. This model is a slight modification of a currently existing, unused model developed for the OU2 HHRA.
[2]Modeling evaluation is continuing at this time and a simple numerical model (using MODFLOW and MT3D) may be constructed.
[3]It is a common practice to perform a steady state flow calibration and then allow the transport simulation to be transient.

Summary of Site-Wide Groundwater Modeling Projects at the Rocky Flats Environmental Technology Site

November 22, 1994

Barry L. Roberts

BLR

Introduction

This document presents a summary of the RFETS site-wide groundwater modeling activities performed over the last several years. A synopsis of the work completed for FY 93 and FY 94 is presented followed by a discussion of issues related to possible future modeling activities. Several figures are included to further illustrate portions of this work.

Fiscal Year 1993 Site-wide Groundwater Modeling Project

During FY 93, a groundwater flow model for the Rocky Flats Environmental Technology Site (RFETS) was developed using in-house resources by what was then the Geosciences Division. This model covered an areal extent that includes all of the RFETS industrial area and a large portion of the RFETS buffer zone (Figure 1). The simulation grid was implemented with a node spacing of 200 feet along rows and columns.

The FY 93 version of the RFETS site-wide flow model focused on the waters in the unconsolidated surficial materials and treated the Rocky Flats Alluvium, hillslope colluvium, and valley fill materials as a single, unconfined layer within the model. The model represented groundwater conditions (head elevations) during the spring of 1992.

The computer code selected for the FY 93 site-wide flow modeling project was the modular, three-dimensional finite-difference groundwater flow model of the U.S. Geological Survey (USGS) commonly referred to as MODFLOW. Although capable of simulating vertical flow, MODFLOW is commonly used to simulate saturated flow in two-dimensional layered systems with varying vertical conductance between the layers.

The results from this preliminary modeling are presented in the 1993 Site-wide Groundwater Flow Modeling Status Report. Products produced from this project include updated site-wide bedrock and groundwater elevation maps, as well as the first calibrated site-wide flow model for the RFETS. The results from this initial effort have highlighted several areas for improving the RFETS site-wide groundwater flow model.

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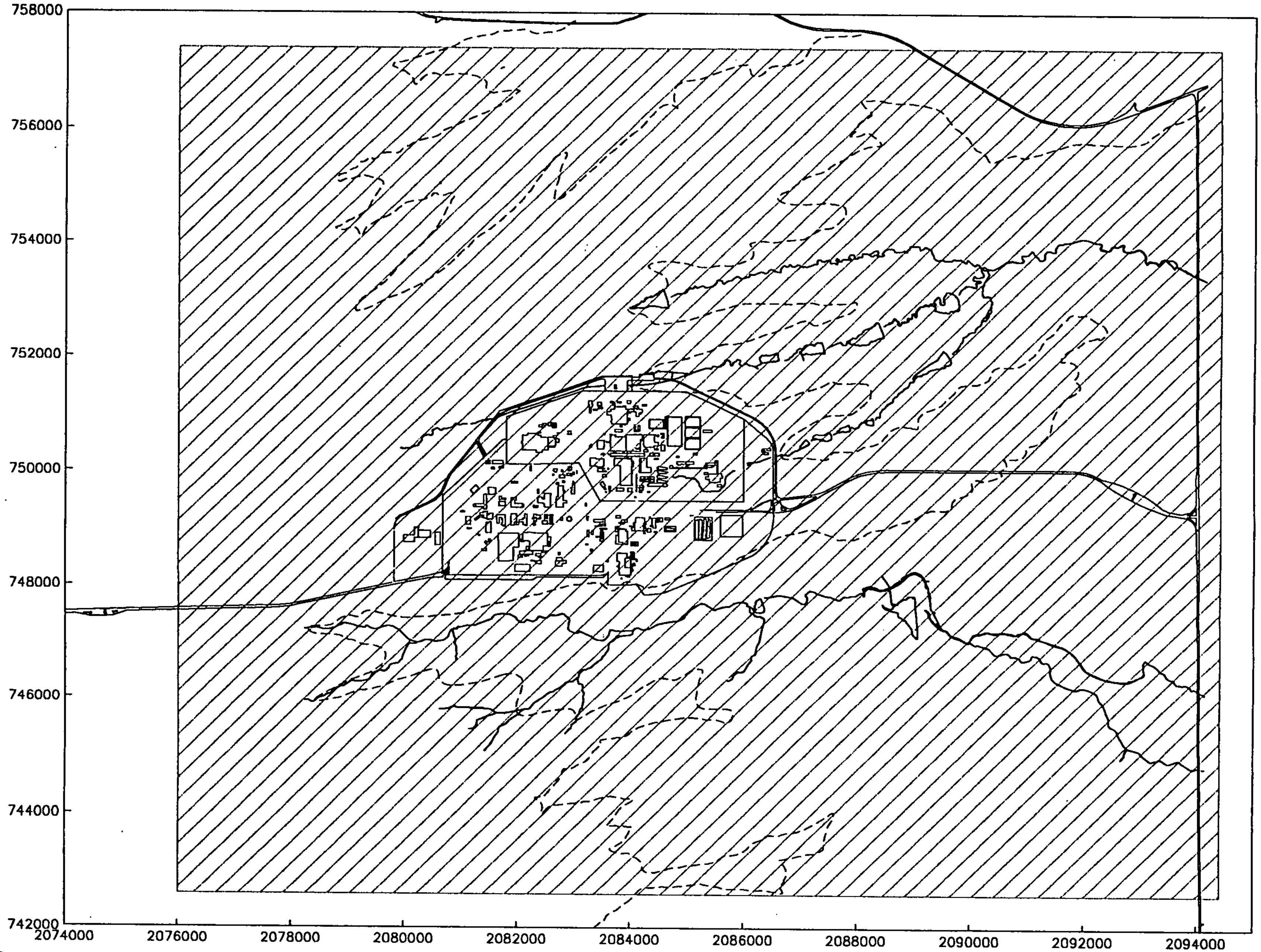

Figure 1
Region covered in FY 93 site-wide groundwater model.

The main features of the FY 93 site-wide modeling project are:

- the model covered the entire industrial area and a majority of the buffer zone
- it focused on saturated groundwater flow in the unconsolidated surficial materials
- a fixed 200 foot grid spacing was used
- groundwater-surface water interactions were included
- the model was calibrated for spring 1992 conditions
- contaminant transport was not included

Fiscal Year 1994 Site-wide Groundwater Modeling Project

The work that was planned for FY 94 involved the expansion and refinement of the FY 93 site-wide flow model, based on recommendations from the FY 93 Site-wide Groundwater Flow Modeling Status Report. The model would cover the same area as the FY 93 model, but with a refined grid spacing, and the incorporation of additional hydrologic features. Results from the FY 94 flow modeling were then used to perform a flow-path analysis for the 1994 Well Evaluation Report (WER). This flow-path analysis would be done using particle tracking and would assist in the evaluation of the current monitoring well network at the RFETS.

Implementation of these enhancements was in progress when direction to change the focus of this work was received from DOE. This DOE request was based on the need for more detailed information within the drainages of Woman and Walnut Creeks. To meet the requests from DOE and the WER commitments, the modeling region was reduced to the hatchured area shown in Figure 2. This area includes an large portion of the Industrial Area, and the two major drainages (Woman Creek and Walnut Creek) that drain the site. A flow model was developed and calibrated for this region. Although this flow model was conceptually similar to the FY 93 flow model (i.e., 2D saturated flow in the surficial materials using MODFLOW), it used a refined grid with variable spacing (from 75 to 200 feet), and added additional features to improve the model calibration.

The results from the flow model were then used to investigate the major groundwater flow paths using particle tracking. Particle tracking involves following the pathway of imaginary

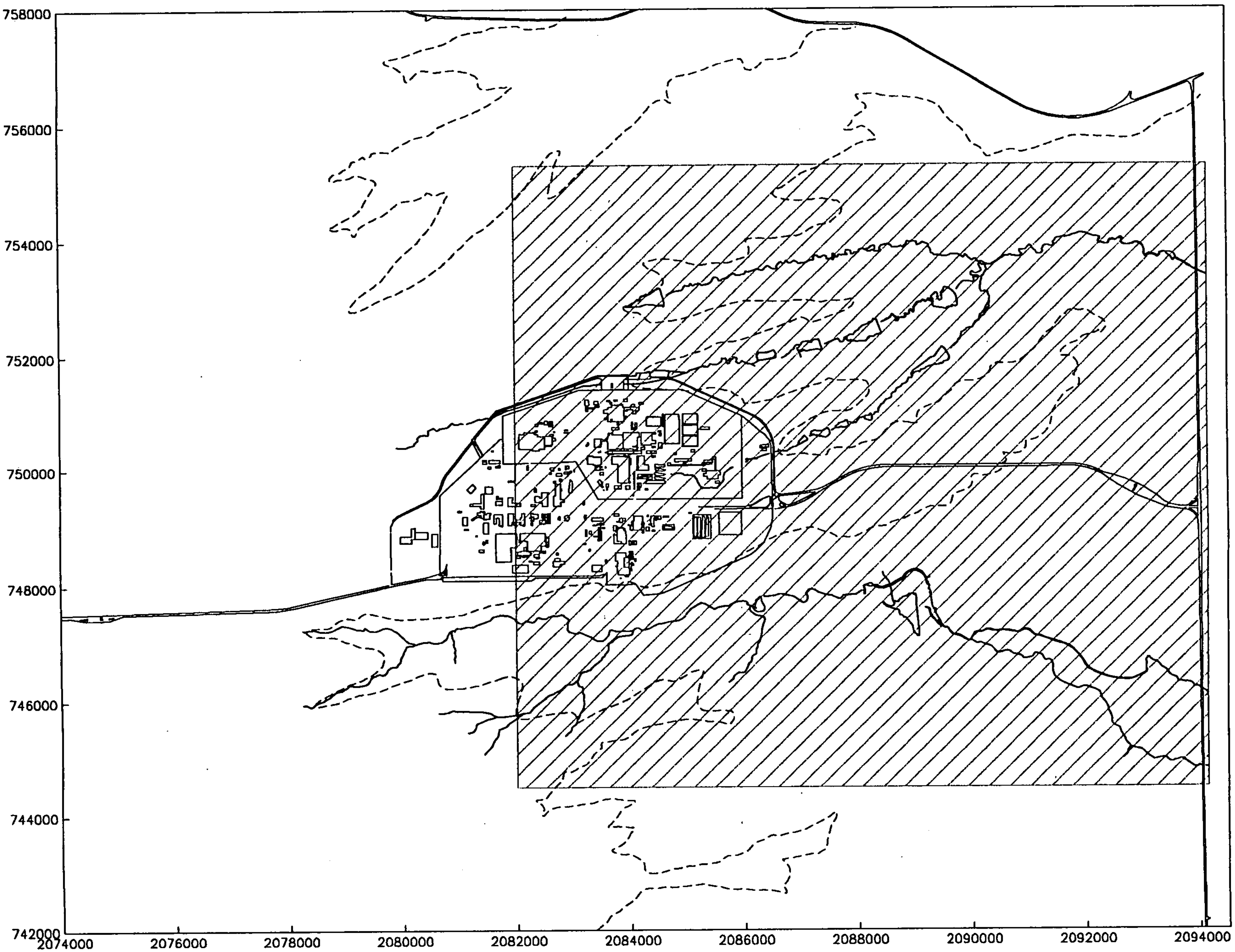

Figure 2

Area of study for WER flow path analysis.

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particles placed within the groundwater flow field. As the particle tracking simulation proceeds, the particles move through the groundwater system based on the groundwater velocities at each model grid node. The information to determine these velocities comes from the groundwater flow model. The particles can be tracked for any length of time. The particle tracking performed for the WER represents 10 years of groundwater movement.

The particle tracking for the WER was done using the PATH3D particle tracking software. PATH3D is a three-dimensional, groundwater flow path and travel-time simulation package. It uses hydraulic conductivity, head distribution, and grid spacing information from a flow model to compute groundwater flux and velocity in each of three-dimensions (x, y, z). There is no retardation of the particles due to interactions with the solid matrix, so the particles travel at the speed of the groundwater. Retarded contaminants would travel at a slower rate than that indicated by the PATH3D output.

The output from the PATH3D analysis was used to evaluate the effectiveness of the present monitoring well network. This was done by using the particle tracking software to project the migration pathways of contaminated groundwater and comparing these pathways against the existing monitoring well network. Suggestions for thirteen additional monitoring locations were made based on this work.

Several figures from the 1994 Well Evaluation Report are included at the end of this section to illustrate this work. Full details and additional figures are in the 1994 Well Evaluation Report.

The main features of the FY 94 flow modeling and particle tracking project are:

- a reduced model domain covering the main industrial area and the Woman and Walnut Creek drainages was used
- it focused on saturated groundwater flow in the unconsolidated surficial materials
- a variable grid spacing from 75 to 200 feet was used
- groundwater-surface water interactions were included
- several sub-surface drain features were included

- the model was calibrated for spring 1992 conditions
- particle tracking representing 10 years of groundwater travel was performed
- contaminant transport was not included

Considerations for Future Work

Several examples of where the continuation of site-wide groundwater modeling would be useful have come to light recently. Most notable are the requirements for the Ecological Risk Assessments for OUs 5 and 6 and the RFETS Comprehensive Risk Assessment. Each of these tasks require groundwater modeling efforts on a scale larger than an individual OU. These needs would be best addressed through site-wide groundwater modeling. The site-wide modeling activities accomplished to date provide an important foundation for any future work.

The next logical step for the continuation of site-wide groundwater modeling activities would primarily be determined by the objectives of the studies at hand. The objectives would determine the size of the region to be modeled, the grid spacing, number of layers, time frame, and general type of the model. Future modeling activities would likely involve additional flow modeling, as well as particle tracking and/or contaminant transport modeling. The additional flow modeling would be needed to update the flow model with information obtained since the last modeling activities.

The dismantling of the Geosciences Division raises additional concerns for the continuation of the site-wide groundwater modeling activities. All of the personnel who were previously involved in the site-wide modeling activities are now distributed across several different OU Closure Groups. Would these personnel be reassigned? Which group would fund this work? Would other ex-Geoscience technical personnel be available for consultation? All of these questions would need to be addressed to some extent when the site-wide groundwater modeling is continued.

EXAMPLE FIGURES FROM THE 1994 WELL EVALUATION REPORT

MEMO

TO: Win Cromec, SME for Risk Assessment, x8576
FROM: Mary A. Siders, Geochemist, Industrial Area OUs, x6933 MAS
DATE: November 18, 1994
SUBJECT: **OVERVIEW OF THE UTILITY AND CURRENT STATUS OF GEOCHEMICAL MODELING AT RFETS**

As agreed to during our meeting last week (November 9), I have prepared a descriptive summary of geochemical modeling that outlines how such modeling could be used at RFETS, and the current status of geochemical modeling at RFETS. Wayne Belcher (OUs 5, 6, and 7, x6931) and Barry Roberts (Industrial Area OUs, x8623) have reviewed and commented on the earlier draft of this summary.

This skeletal overview of geochemical modeling describes the types of geochemical models currently available, the value of geochemical modeling, the data requirements and limitations of geochemical modeling, the potential application of such modeling at RFETS, and the current status of geochemical modeling at RFETS.

If you require more detailed discussion on any aspect of geochemical modeling and assessment, please feel free to make such a request. Although I am assigned to the Industrial Area OUs and they are generally my first priority, I am here to offer technical support to any of the staff of Environmental Restoration Division. Policy decisions on technical issues impact all individual OUs, so it is generally best to be proactive in establishing the most credible technical policy we can to support our client.

cc: W.R. Belcher
B.L. Roberts
B.D. Peterman
R.S. Roberts
M.L. Hogg

11-18-94

GEOCHEMICAL MODELS

Using thermodynamic data, geochemical computer models mathematically describe the chemical reactions that control the chemistry of a natural water. These models predict the aqueous chemistry that should exist under equilibrium conditions in a variety of groundwater environments.

TYPES OF GEOCHEMICAL MODELS

Three basic types of calculations are used to describe the geochemistry of the groundwater system:

(1) **Speciation calculations** provide the basis for a measure of the tendency of a particular mineral to dissolve or precipitate under a given set of conditions.

(2) **Mass-balance calculations** constrain the chemistry of groundwater along the flow path, based on the conservation of mass.

(3) **Mass-transfer calculations** employ thermodynamic data to predict solution composition and transfers between the aqueous, solid, and gaseous phases in a system.

VALUE OF GEOCHEMICAL MODELING

(1) Geochemical modeling quantifies the effects of temperature, ionic strength, solution composition, and reduction-oxidation (redox) conditions on ion speciation, mineral solubility, and sorption of aqueous species.

(2) Geochemical modeling illustrates which reactions control the solubility of different chemicals, which processes are dominant in a complex aqueous system, and the relative importance of competing chemical processes.

(3) Ion speciation determined by geochemical modeling can be used to interpret bioavailability and acute toxicity data. (The general assumption is that uncomplexed metals tend to have higher biological potency).

(4) Geochemical models support risk assessment, especially in assessing the relative toxicity and mobility of chemicals. Toxicity and mobility vary with redox state, pH, and solution composition; all of which affect the speciation and complexation of chemicals. Modeling defines these properties in a given environment; examples include the toxicity of chromium (Cr^{+3} versus Cr^{+6}), and the mobility of uranium (U^{+4} versus U^{+6}).

DATA REQUIREMENTS FOR GEOCHEMICAL MODELING AT RFETS

Most of the requirements for geochemical modeling at RFETS have been met, including:

(1) Data for analytical chemistry, including major-ion and trace element abundances
(2) Field-measured pH, water temperature, and specific conductivity
(3) Mineralogic data for type, composition, and relative abundance of phases in bedrock.

However, more data are needed for:

(1) Redox conditions in groundwater across the site. (Redox must be measured in the field, using a flow-through cell that avoids atmospheric exposure of the sample).
(2) Mineralogy of unconsolidated ("surficial") geologic materials (i.e., Rocky Flats Alluvium, colluvium, and valley-fill alluvium).
(3) Empirically determined distribution coefficients (K_d) for modeling sorption and for determining contaminant retardation for contaminant-transport modeling.

POTENTIAL APPLICATION OF GEOCHEMICAL MODELING AT RFETS

RISK ASSESSMENT

Use to help determine toxicity and mobility of chemicals, by determining the likely chemical form of each inorganic constituent. The form affects the bioavailability, the toxicity, and the mobility of the constituent. Apply to risk assessments for each OU.

CERCLA OU INVESTIGATIONS

Use modeling to assist in interpreting analytical data gathered during RI/FS investigations in each OU. Again, an understanding of the geochemical environment helps to predict the speciation, mobility, and transport rates for inorganic constituents. "What if" scenarios can be created by adjusting Eh, pH, and solution chemistry in the model, to determine the effect of such changes on the contaminants of interest.

RCRA UNITS

Geochemists can work with transport modelers to predict the fate and transport of inorganic constituents in identified contaminant plumes. The behavior of the contaminants is a function of speciation and rock/water interactions under the specific conditions of a particular geochemical environment.

COMPREHENSIVE, INTEGRATED OVERVIEW OF RFETS (DOE Order 5400.1)

Determine the evolution of groundwater chemistry along sitewide flow paths, examine surface-water/sediment and groundwater/rock interactions. Determine concentrations expected on the basis of equilibrium solubility with respect to certain solid phases.

ASSUMPTIONS AND LIMITATIONS OF GEOCHEMICAL MODELS

(1) Geochemical models rely on the assumption that equilibrium conditions are achieved between the aqueous and solid phases. However, low-temperature aqueous systems are not usually at equilibrium.

(2) Models ignore reaction kinetics, which may constrain the rate of reaction.

(3) Most models do not adequately model organic chemistry, and the models ignore biological processes.

CURRENT STATUS OF GEOCHEMICAL MODELING AT RFETS (11-15-94)

Data for all groundwater wells at RFETS, for the period 1990 through first quarter of 1994, have been compiled and cleaned, and summary statistics for groundwater chemistry at each well have been computed. (These data reside as SAS files in the computers of M.A. Siders).

Values of the mean concentrations of major and trace elements for selected wells have been input for WATEQF and NETPATH modeling. Results and interpretation of this modeling are provided in Volume III of the Sitewide Characterization Studies — the *1994 Groundwater Geochemistry Report* — and are summarized below.

Aqueous chemistry of groundwater in wells along four flow paths was modeled using WATEQF (speciation) and NETPATH (mass-balance) models. Results of this modeling indicate that the chemical evolution in groundwater chemistry across the site:

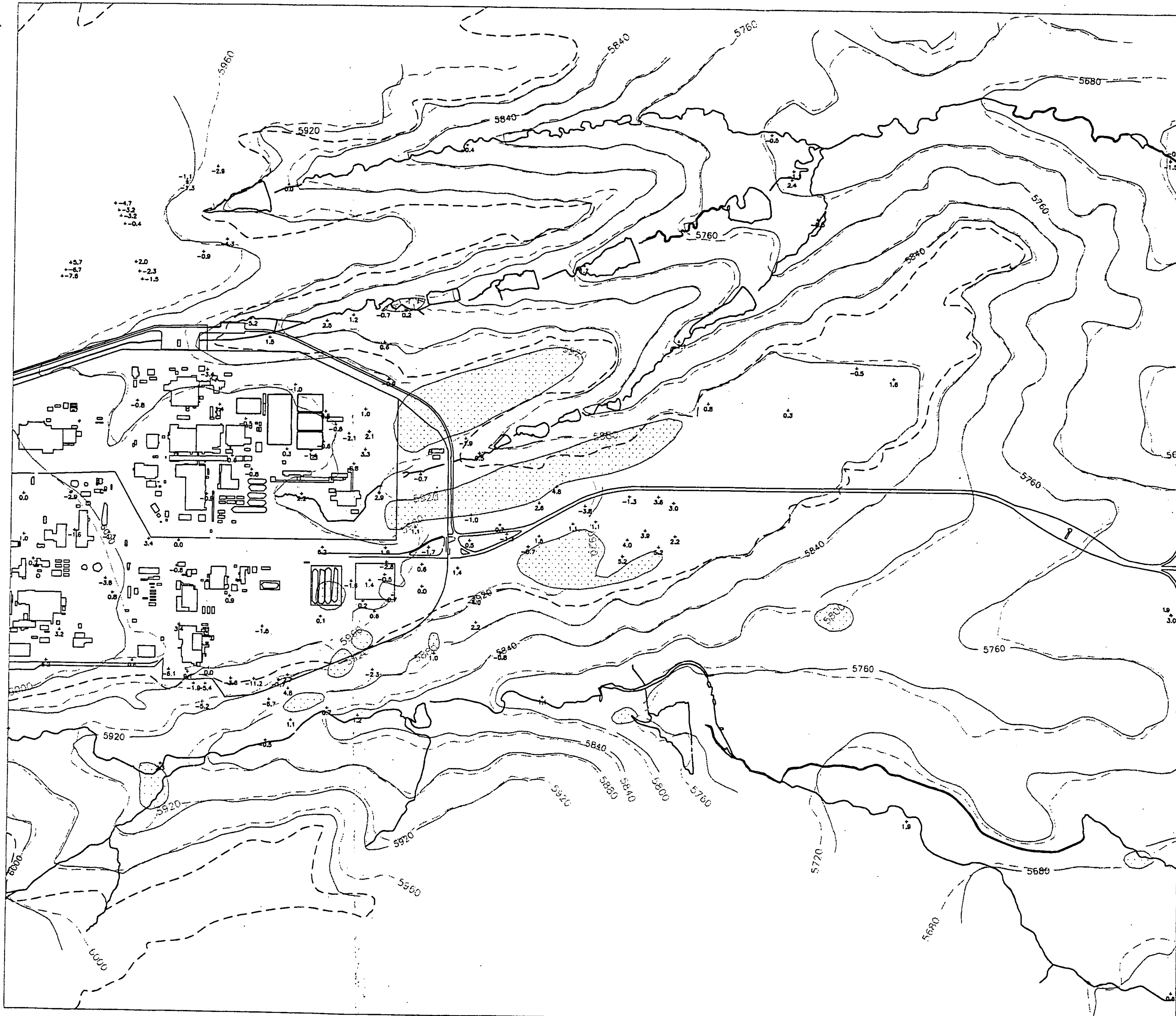
(1) produces approximately one-order-of-magnitude increase in the concentrations of inorganic constituents as groundwater traverses from west to east across the entire site,

(2) does not require the addition of contaminant recharge to generate the composition of the "final" water from that of the "initial" water,

(3) suggests that the "background" composition of groundwater, as defined in the 1993 Background Geochemical Characterization Report, may suffer from an "upgradient bias",

(4) shows that background concentrations are greater than established water standards for some metals and radionuclides; and that equilibrium solubility with respect to some minerals for some constituents will maintain concentrations above some of the current groundwater standards, and

(5) shows that the chemistry of water is locally impacted in the Industrial Area of RFETS, but, currently, the contamination is largely attenuated by the time groundwater reaches the eastern boundary of RFETS.



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Rocky Flats

Environmental Technology Site

Simulated and Observed Groundwater Elevations

LEGEND

Contour Based on Observed Groundwater Elevations

Contour Based on Flow Model Results

Contour Interval 40 feet

3.0 Calibration Error

Surface Water Feature

Extent of Rocky Flats Alluvium

Desaturated Area

Attachment 1
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TN

12'

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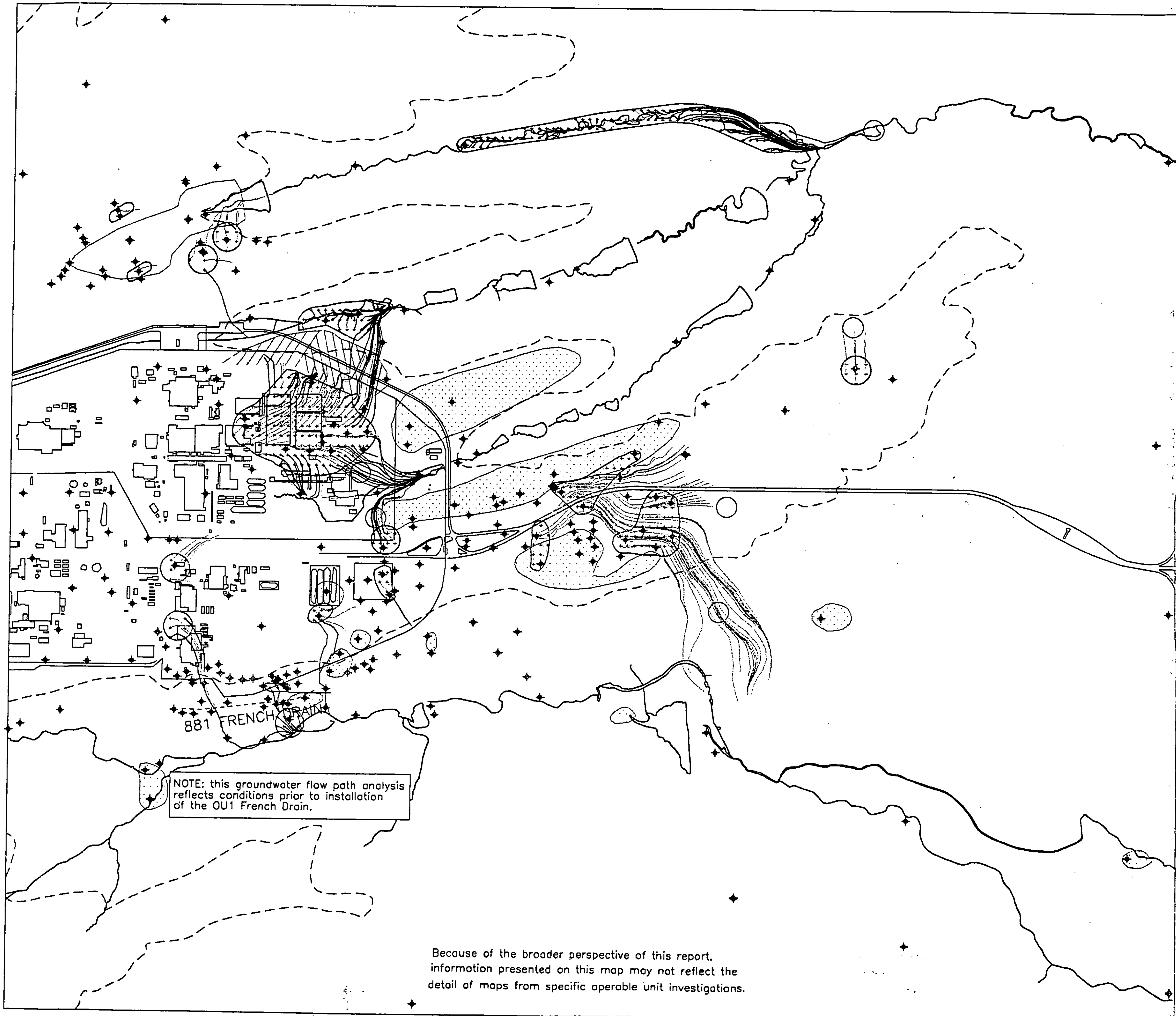
FEET

State Plane Coordinate Projection

1994 Well Evaluation Report

Figure 4-9

Date: August 15, 1994



U.S. Department of Energy
Rocky Flats
Environmental Technology Site

Nitrate plus Nitrite 2nd Quarter 1992

PARTICLE TRACE LEGEND

- Contamination Extent From 1993 Well Evaluation Report
- Complete 10 Year Particle Track
- Final Particle Position in Stream at or Before 10 Years
- Particle Captured by Drain or Trapped at Cell at or Before 10 Years
- Number of Tracking Steps Exceeded
- Possible Future Monitoring Site
- Existing Alluvial Monitoring Well
- Surface Water Feature
- Subsurface Drain
- Extent of Rocky Flats Alluvium
- Unsaturated Area

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State Plane Coordinate Projection

1994 Well Evaluation Report
Figure 7-12

Date: September 16, 1994

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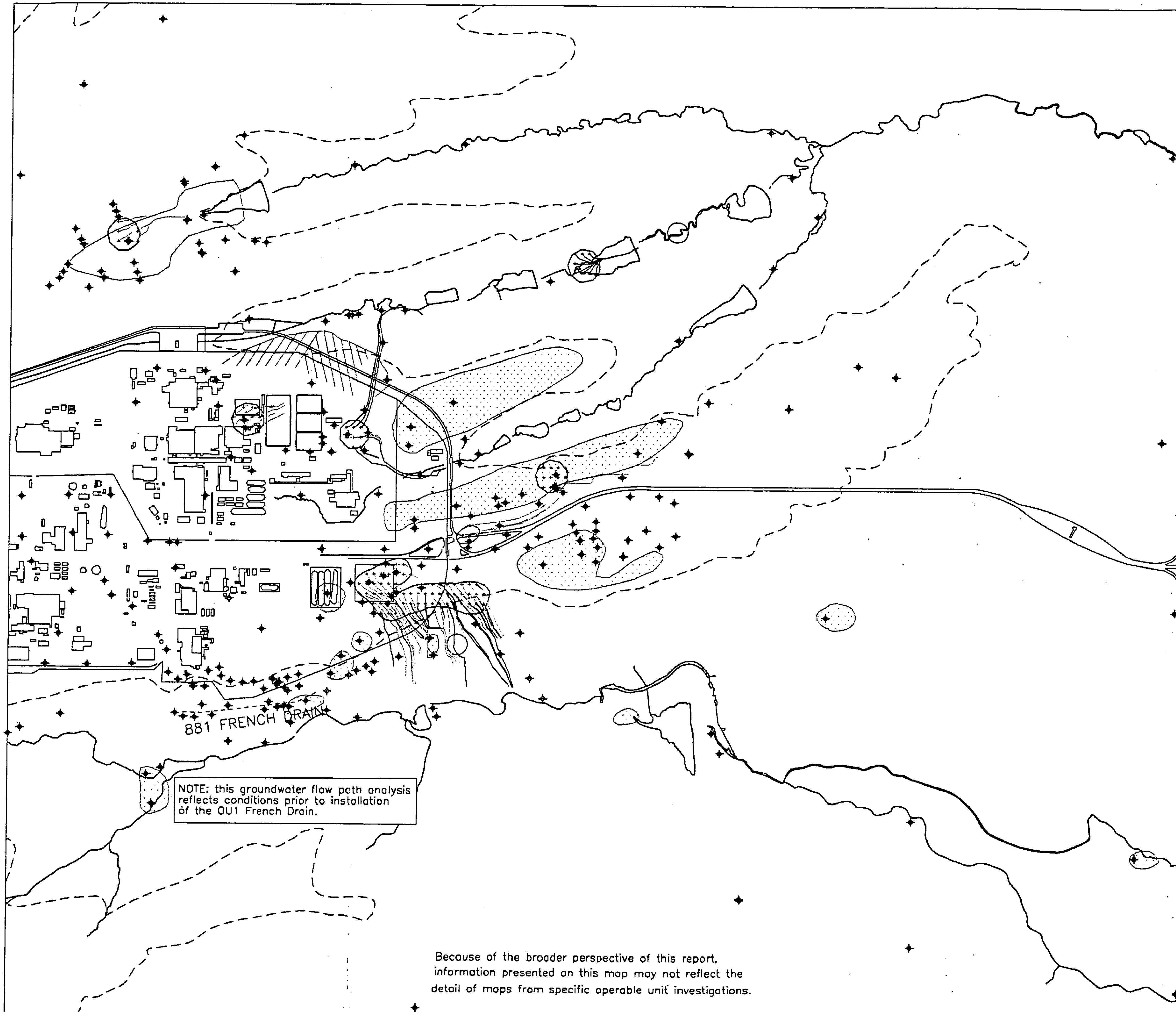

U.S. Department of Energy
Rocky Flats
Environmental Technology Site

Americium-241
2nd Quarter 1992

PARTICLE TRACE LEGEND

Contamination Extent From 1993 Well Evaluation Report

Complete 10 Year Particle Track

Final Particle Position in Stream at or Before 10 Years

Particle Captured by Drain or Trapped at Cell at or Before 10 Years

Number of Tracking Steps Exceeded

Possible Future Monitoring Site

Existing Alluvial Monitoring Well

Surface Water Feature

Subsurface Drain

Extent of Rocky Flats Alluvium

Unsaturated Area

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State Plane Coordinate Projection

1994 Well Evaluation Report
Figure 7-13

Date: September 16, 1994

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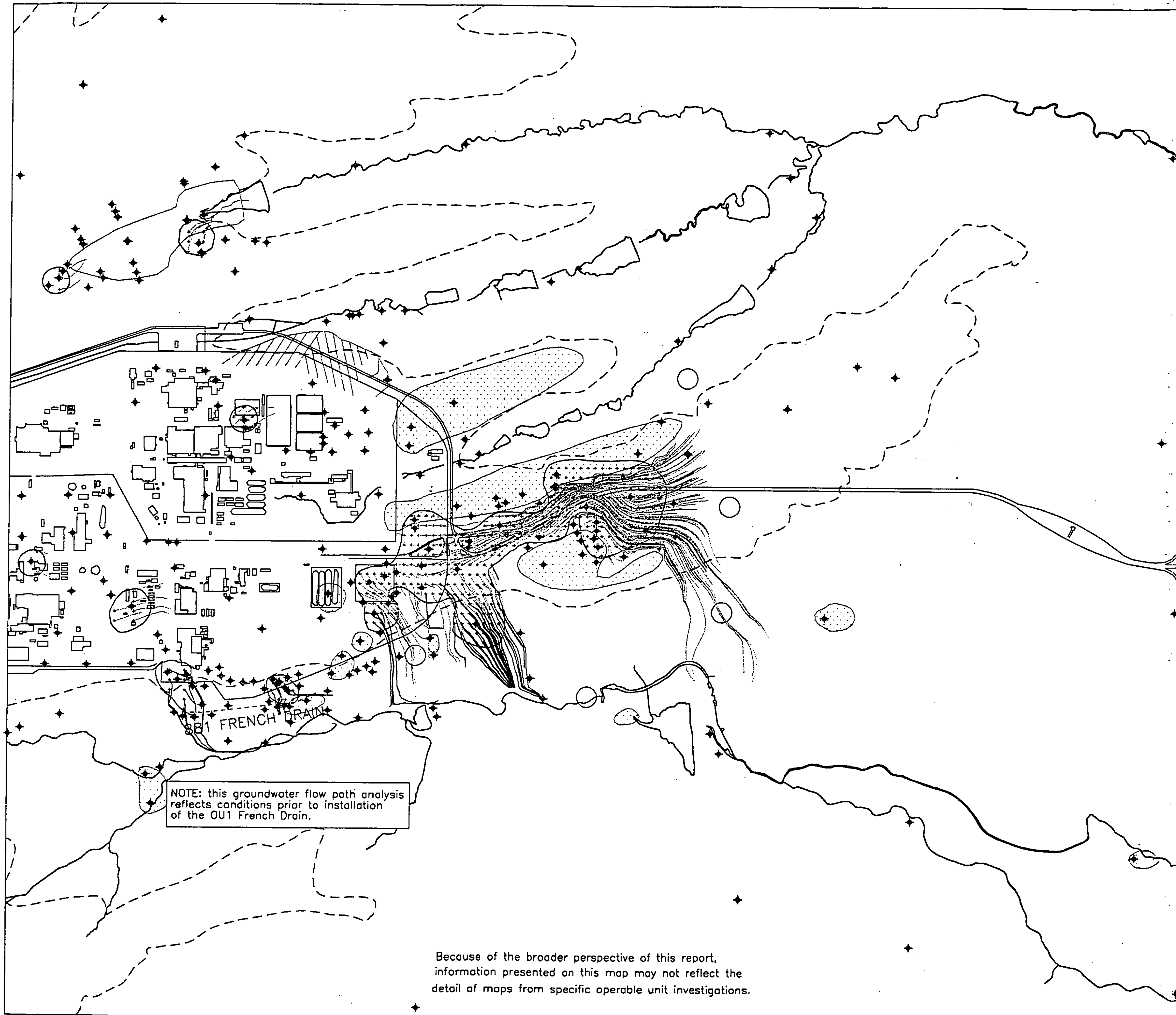

Because of the broader perspective of this report, information presented on this map may not reflect the detail of maps from specific operable unit investigations.

U.S. Department of Energy
Rocky Flats
Environmental Technology Site

Average Tetrachloroethene Average 1989 – 1993

PARTICLE TRACE LEGEND

- Contamination Extent From 1993 Well Evaluation Report
- Complete 10 Year Particle Track
- Final Particle Position in Stream at or Before 10 Years
- Particle Captured by Drain or Trapped at Cell at or Before 10 Years
- Number of Tracking Steps Exceeded
- Possible Future Monitoring Site

- Existing Alluvial Monitoring Well
- Surface Water Feature
- Subsurface Drain
- Extent of Rocky Flats Alluvium
- Unsaturated Area

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State Plane Coordinate Projection

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1994 Well Evaluation Report
Figure 7–14

Date: September 16, 1994

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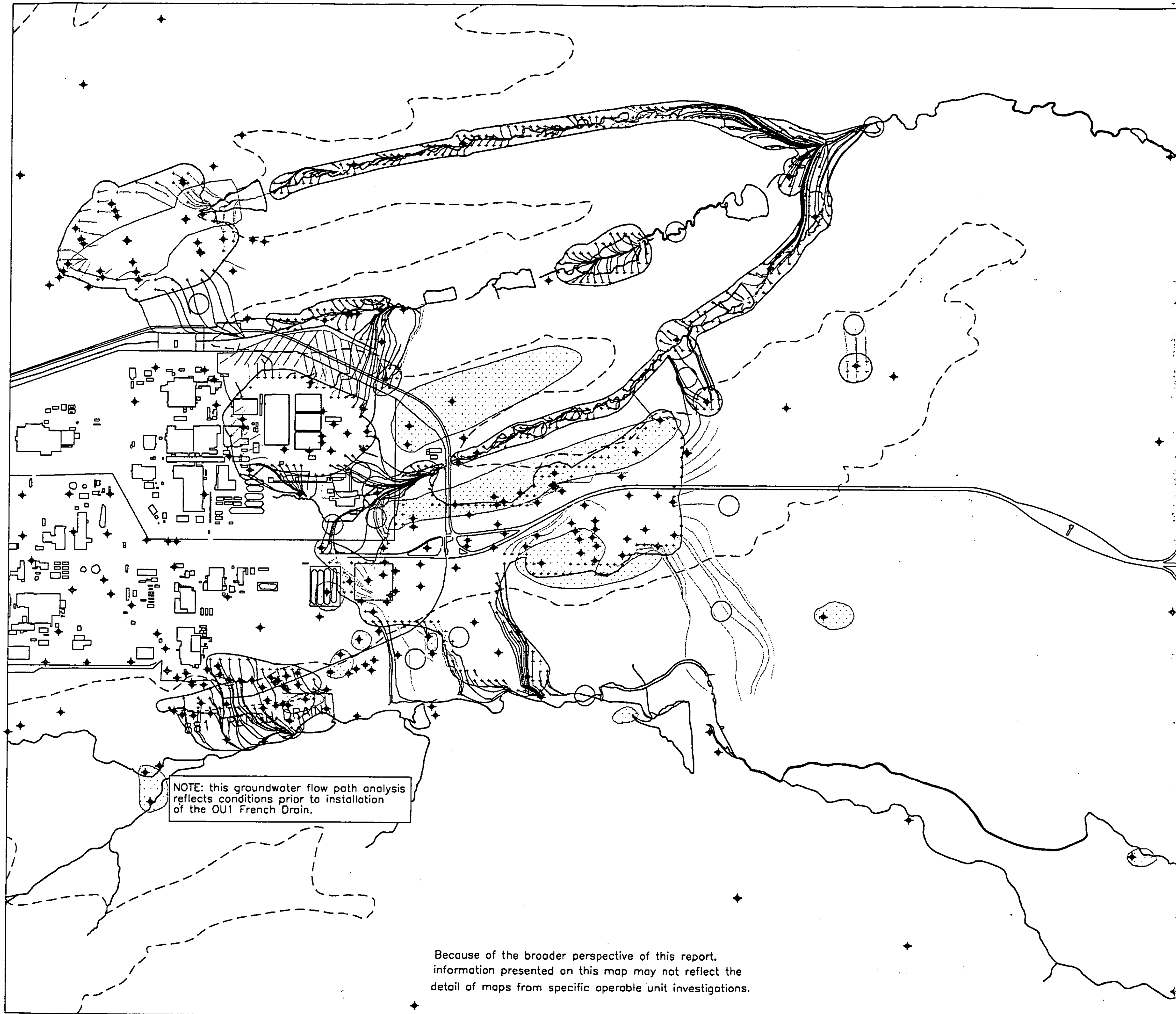

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Rocky Flats
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Composite Contaminant Extent

PARTICLE TRACE LEGEND

Contamination Extent From 1993 Well Evaluation Report
Complete 10 Year Particle Track
Final Particle Position in Stream at or Before 10 Years
Particle Captured by Drain or Trapped at Cell at or Before 10 Years
Number of Tracking Steps Exceeded
Possible Future Monitoring Site

Existing Alluvial Monitoring Well
Surface Water Feature
Subsurface Drain
Extent of Rocky Flats Alluvium
Unsaturated Area

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State Plane Coordinate Projection

1994 Well Evaluation Report
Figure 7-16

Date: September 16, 1994

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